Strictly localized eigenstates on a three-dimensional Penrose lattice

Marian Krajčí* and Takeo Fujiwara
Department of Applied Physics, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113, Japan
(Received 23 June 1988)

The existence of the strictly localized states in a three-dimensional (3D) Penrose lattice is demonstrated for a simple tight-binding model. In the center model there exist degenerate states at an energy $E=2$; the corresponding wave functions are strictly localized and have the form of tenfold rings. In the vertex model the degenerate states at $E=0$ were found; the corresponding wave functions have the form of rhombitriaconta icosidodecahedra. The degeneracy of these states is proportional to the system size and, therefore, is infinite in the infinite system.

I. INTRODUCTION

Quasicrystals, quasiperiodic systems with a long-range bond-orientational order, attract wide interest from the viewpoint of both experimental and theoretical physics. Since the successful preparation of real samples of these interesting systems, quasicrystals pose a challenge to those who attempt to understand their structure and their physical properties. Quasicrystals are solids with much more general and more complicated arrangements of atoms than we have considered so far. Though many experimental and theoretical works devoted to the investigation of the structure of quasicrystals have appeared in print, the local arrangement of atoms in real systems is not yet fully understood. One possible approach to understanding the structure of real quasicrystals is to consider their atomic structure as a certain decoration of a three-dimensional (3D) Penrose lattice (PL).

The prerequisite for understanding the physical properties of quasicrystals is a knowledge of their electronic structure. The electronic structure of realistic models of quasicrystals has not been yet calculated, mainly because of our lack of information about detailed positions of the atoms in the system. However, even a very simple model of quasicrystals based on the decoration of the 3D Penrose lattice by one atom with one s orbital can elucidate the possibility of exotic physical properties of quasicrystals caused by their quasicrystalline nature.

The electronic structure of 1D quasilattices (Fibonacci lattices)[1,2] and 2D Penrose lattices have been investigated by several authors.[3-6] The energy spectrum of a 1D quasilattice is known to be singular continuous. The peculiar features of the electronic structure of 2D Penrose lattices are the exotic (multifractal) character of the energy spectrum, the existence of the infinitely degenerated energy levels, and the strictly localized (confined) and string states corresponding to this level.

The electronic structure of 3D Penrose lattices were calculated,[7] and an electronic structure with similar character to those of crystal lattices was reported.

The quasiperiodicity follows from the golden mean $\tau=(1+\sqrt{5})/2$ which plays a central role in quasilattices with icosahedral bond-orientational order. In the numerical calculations of the electronic structure, as the system is nonperiodic, we should impose the Dirichlet boundary conditions or treat a small finite system. Because of the sensitivity of the electronic structure on boundary conditions, the most natural way to get a well-defined model is imposing optimal periodic approximation to the nonperiodic system. The systematic procedure for constructing "periodic quasilattices" consists in replacing the golden mean τ by its rational approximation[3,8] $\tau_n=F_{n+1}/F_n$. F_n is a Fibonacci number, defined as $F_{n+1}=F_n+F_{n-1}$ for $n\geq 1$ with $F_0=0$ and $F_1=1$. For $n=0,1,2,3,\ldots$, we get a series of periodic quasilattices with increasing periods. For large n the generated structure tends to the true Penrose lattice. We call these structures the "periodic" Penrose lattices (PPL's).

In this work we investigated the electronic structure of simple 3D models of quasicrystals. We demonstrate the existence of the strictly localized states in 3D Penrose lattices. The basis of the structural models is PPL's consisting of the golden rhombohedra. In Sec. II some details of the construction are given. We considered two types of the decoration of PPL's by atoms. In the vertex model, the atoms are placed on the vertices of the rhombohedra; in the center model, the atoms are placed at the centers of the rhombohedra. We considered one s orbital per atom. The Schrödinger equation of the system is

$$\sum_j t_{ij}\psi_j=E\psi_i \ . \tag{1.1}$$

The transfer-matrix element t_{ij} is assumed to be nonzero only between the nearest neighbors and constant $t_{ij}=-1$. The eigenvalues and eigenvectors were calculated by the exact diagonalization. The resulting electronic structure is presented in Sec. III. The results are discussed in Sec. IV.

II. STRUCTURAL MODELS

The structural models of 3D Penrose lattices were generated by the dual method.[9,10] In the dual space, the icosahedral basis set $\mathbf{g}_l=\{0,1,\tau_n\}_{\text{c.p.}}$ for $l=1,2,3$ and $\mathbf{g}_l=\{0,-1,\tau_n\}_{\text{c.p.}}$ for $l=4,5,6$ were chosen as grid vectors, c.p. stands for cyclic permutation. τ_n is the rational approximation to the golden mean. The grid vectors defines the hexagrid of planes G_6,

$$G_6=\{\mathbf{x}\in E^3|\mathbf{x}\cdot\hat{\mathbf{g}}_l-\gamma_l=k_l|\mathbf{g}_l|;\ l=1,\ldots,6;\ k_l\in\mathbb{Z}\}\,, \tag{2.1}$$

where $\hat{\mathbf{g}}_l=\mathbf{g}_l/|\mathbf{g}_l|$. The parameters γ_l defining the shift of the origin are chosen to get the regular grid. Any one point intersects no more than three planes. Each intersection point x_0 defines in the real space the rhombohedron with the vertices

$$\mathbf{R}(\mathbf{x}_0,j)=\sum_i K_i(\mathbf{x}_0+\boldsymbol{\varepsilon}_j)\mathbf{t}_i,\quad j=1,2,\ldots,8 \tag{2.2}$$

where $K_i(\mathbf{y})$ is an integer function,

$$K_i(\mathbf{y})=[(\mathbf{y}\cdot\hat{\mathbf{g}}_i-\gamma_i|)/|\mathbf{g}_i|],\quad i=1,2,\ldots,6 \tag{2.3}$$

which in a small neighborhood of the intersection point $\mathbf{x}_0$ takes eight values $K_i(\mathbf{y}_j)$, $j=1,2,\ldots,8$, corresponding to eight subspaces determined by the intersecting planes, $\mathbf{y}_j=\mathbf{x}_0+\boldsymbol{\varepsilon}_j$; the infinitesimal vectors $\boldsymbol{\varepsilon}_j$ define the subspaces. $\mathbf{t}_i$ are the tiling vectors. We chose $\mathbf{t}_i=\hat{\mathbf{g}}_i$ with τ_n here and only here equal to the exact golden mean τ.

If τ_n takes in the dual (grid) space values F_{n+1}/F_n for certain n, we get the periodic Penrose lattice. The lattice has bcc symmetry for $n=1,4,7,\ldots,3k+1,\ldots$, and for other n it has simple cubic (sc) symmetry. The period of the cubic symmetry is $d_n=(2+2/\sqrt{5})^{1/2}\tau^n$. The cubic cell consists of $N_n=4F_{3n+3}$ golden rhombohedra: $4F_{3n+2}$ of them are prolate and $4F_{3n+1}$ oblate. We will refer to the models by the pair of corresponding Fibonacci numbers (F_{n+1},F_n).

We constructed three models of PPL's: (2,1), (3,2), and (5,3), consisting of 136, 576, and 2440 golden rhombohedra, corresponding to $n=2$, 3, and 4, respectively. The parameters γ_l were chosen as $\gamma_l=0.5+l\times10^{-4}$, $l=1,\ldots,6$.

III. ELECTRONIC STRUCTURE

A. The center model

In the center model, atoms are placed at the centers of the rhombohedra. The Hamiltonian matrix element is nonzero only between the centers of the neighboring rhombohedra with a shared face. The coordinate number of each atom is equal to 6.

The calculated integrated densities of states $N(E)$ and the eigenvalue distribution $n(E)$ of the biggest model, (5,3), are presented in Fig. 1. The plotting interval for $n(E)$ is 0.08. We prefer the term "eigenvalue distribution" to the common term "density of states," as the density of states in the case of quasiperiodic systems need not be a well-defined quantity.[3]

The spectrum extends from the energy $E=-6.0$ (corresponds to the uniform state $\psi_i=1$) to the energy $E\doteq3.59$. Above this energy there are no states because the odd-membered rings dominate the ring statistics and cause strong frustration in the phase of the wave functions. The steps on the integrated density of states $N(E)$ near the edge of the band is the effect of the finiteness of the system. The integrated density of states of smaller calculated systems, (3,2) and (2,1), are very similar; however, the effect of the finiteness in these systems is more evident.

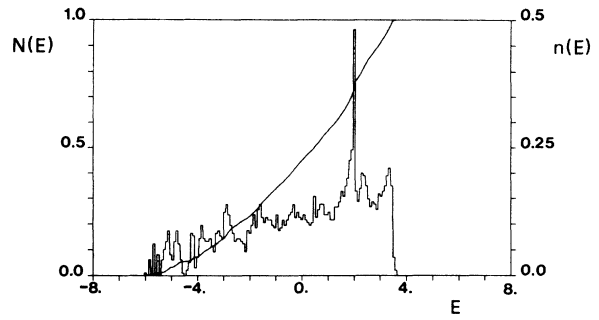

FIG. 1. The integrated density of states $N(E)$ and the eigenvalue distribution $n(E)$ of the (5,3) PPL center model. The plotting interval for $n(E)$ is 0.08. The energy level at $E=2$ is multiply degenerate. The concentration of the eigenvalues around the degenerate level is strongly enhanced.

The peculiarity of the spectrum is the existence of degeneracy at the energy $E=2$. The numbers of the degenerate states of the models are zero, four, and twelve for $n=2$, 3, and 4, respectively. The wave functions of the degenerate states are strictly localized. The wave function is nonzero only on the sites forming tenfold rings. These are shown in Fig. 2. The wave function on each ring has a constant amplitude and its sign is alternating. The number of rings corresponds to the number of degen-

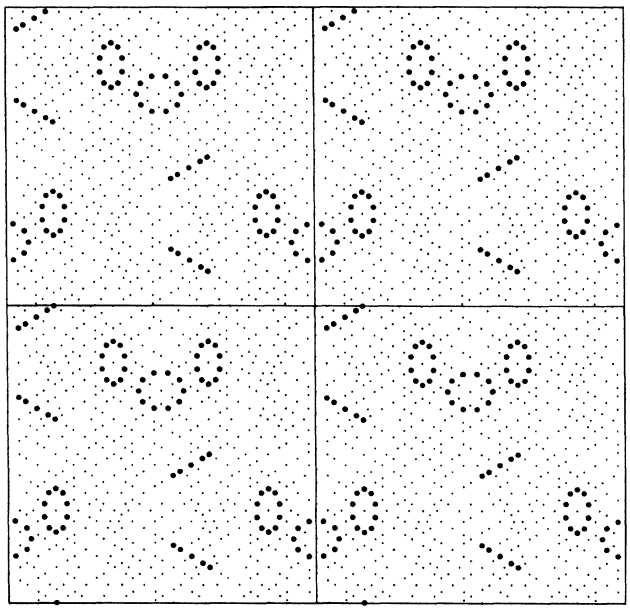

FIG. 2. The projection of the positions of atoms of four cubic cells of the (5,3) PPL center model on the x-y plane, shown by small crosses. The wave function corresponding to the degenerate level $E=2$ is strictly localized. It is nonzero only on the sites forming tenfold rings (solid circles). The wave function has on the ring a constant amplitude and alternating sign. In the (5,3) model there are 12 rings in the cubic cell corresponding to the 12-fold degeneracy. In the figure some of the rings are projected on the same place.

erate states. The rings are separated. Each ring itself is a solution of Eq. (1.1). The structure of the ring is shown in Fig. 3, in which ten oblate rhombohedra are aligned around one common edge—the perpendicular axis of the ring.

B. The vertex model

In the vertex model the atoms are located on the vertices of rhombohedra. The Hamiltonian matrix element is nonzero only between atoms connected by the edge of one rhombohedron. The coordination number varies from 4 to 12. The average coordination number is exactly 6.0.

The calculated integrated density of states $N(E)$ and the eigenvalue distribution $n(E)$ for the largest calculated model, (5.3), are presented in Fig. 4. The plotting interval for $n(E)$ is 0.08. The spectrum is symmetric and extends in the range $E \doteq \pm 6.60$. This range is determined by the average coordination number and its dispersion. The global similarity of the spectrum with that of a simple-cubic lattice is remarkable. The difference comes from the eighth or higher moment of the spectrum. The most interesting feature of the spectrum is the degenerated levels at the energy $E=0$, which we have found in the (5,3) model—the largest investigated model thus far but not in the smaller ones. The level $E=0$ degenerates twice in the (5,3) model. The corresponding wave functions are strictly localized (see Fig. 5). The eigenstates are nonzero only on sites which form together a bcc packing of rhombitriaconta icosidodecahedra (RTID). Each degenerate state forms a sc sublattice of connected RTID. The amplitude of the eigenfunction is constant on one sublattice. Inside each RTID the amplitude of the wave function is zero. The RTID have icosahedral symmetry. Each

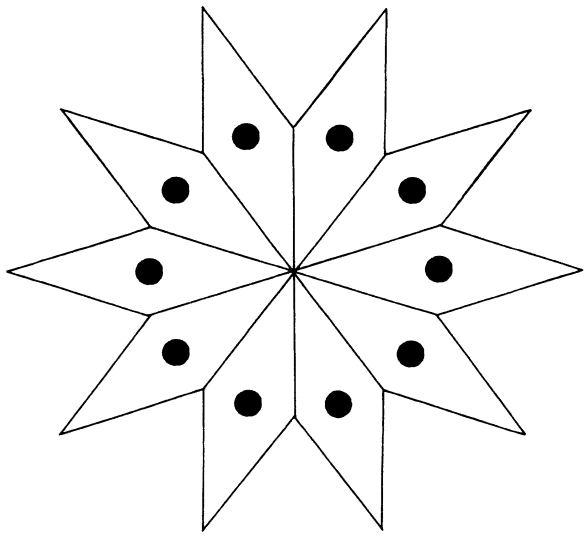

FIG. 3. The structure of the ring from Fig. 2 (the center model) viewed from the top. Ten oblate rhombohedra are aligned around the common edge—the perpendicular axis of the ring. This ring can exist also in the infinite Penrose lattice, which has an infinite degeneracy at $E=2$.

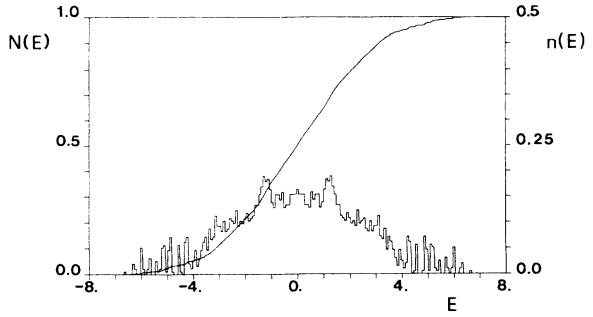

FIG. 4. The integrated density of states $N(E)$ and the eigenvalue distribution $n(E)$ of the (5,3) PPL vertex model. The plotting interval for $n(E)$ is 0.08. The (5,3) model has degenerated twice at the $E=0$ level.

RTID has 120 vertices, 180 edges, and 62 faces. The faces have an even number of edges. There are three types of faces: squares, hexagonals, and decagonals. The sign of the wave function around a face alternates. The edges of RTID are formed by the connection of the second-nearest-neighboring vertices of the 3D Penrose lattice. The length of edges are equal to the length of the diagonals of one golden rhombohedron face:

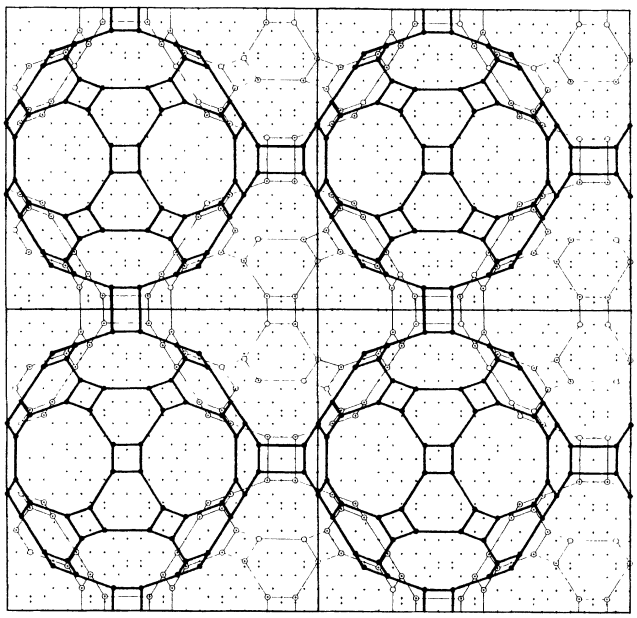

FIG. 5. The projection of the position of the atomic sites of four cells of the (5,3) PPL vertex model on the x-y plane, shown by small crosses. The wave function correspond to the degenerate level $E=0$ is nonzero only on the sites (circles) which together form vertices of the rhombitriaconta icosidodecahedra (RTID). The supporting structure of one degenerate state (solid circles)—the vertices of RTID—is connected by thick lines. The supporting structure of the other degenerate state (open circles) is connected by thin lines. In the extended cubic lattice the wave function corresponding to each degenerate state forms the connected simple-cubic lattice of RTID. Both degenerate states together form the interlocked structure of bcc-packed RTID in the extended cubic lattice.

$(2+2/\sqrt{5})^{1/2}$ and $(2-2/\sqrt{5})^{1/2}$, respectively. The RTID of one sc sublattice are connected through the square faces by the bridges of the length $(2+2/\sqrt{5})^{1/2}$. Both sc sublattices form an interlocked bcc lattice. The bcc structure is obviously the consequence of the bcc symmetry of the (5,3) PPL lattice of our largest structural model.

IV. DISCUSSION

The difficulty in the calculation of the electron structure of quasicrystals is in the necessity of exact diagonalization of very large matrices. This problem is particularly serious in 3D systems. The recursion method does not here give enough information about the spectrum. The largest model we investigated—the (5,3) model—consists of 2440 rhombohedra, and the next one—the (8,5) model—would consist of 10 366 rhombohedra. For such size, special methods for diagonalizing sparse matrices should be used.

On the basis of our calculations we now discuss our observations.

In both models we could not observe any particular characteristics of quasiperiodicity in the spectrum, presumably partly because the size of the models is too small.

The number of the strictly localized states depends on the values of the parameters γ_l.

In the center model the localized states consist of tenfold rings. As the supporting structure (Fig. 3) does not violate the matching rules for 3D Penrose lattices,[11] such states certainly exist in 3D PL's (infinite system). According to Conway's theorem,[12] if a certain structure exists in one place, there is an upper bound of distances to find the exact copy of the structure in another place. The number of such structures is therefore proportional to the volume of the system. In the infinite center model infinite degeneracy therefore exists at $E=2$. In larger models we may expect an existence of other types of localized states; for instance, the string states similar to those observed in 2D models.[4]

The strictly localized states give a δ-function contribution to the energy spectrum. Therefore, the height of the peak of the eigenvalue distribution (Fig. 1) at $E=2$ depends on the plotting interval. At the present value of the plotting interval, 0.08, the degenerate states themselves contribute to the height of the peak only by about 13%. This fact indicates that the concentration of the eigenvalues around the degenerate level is strongly enhanced. The asymmetry of this enhancement, obvious in Fig. 1, is also remarkable.

The degenerate states of the vertex model consist of RTID. The RTID are separable—each RTID itself is a solution of Eq. (1.1). As the internal structure does not have the icosahedral symmetry that the surface has, it is difficult to prove adherence to or violation of the matching rules inside the RTID. However, we have found that at least the structure with the topologically equivalent surface—RTID and more symmetrical internal structure—does not violate the matching rules for 3D PL's. The construction of such structure is indicated in Fig. 6. The structure is built from a rhombic triacontahedron in the center covered by two layers of rhombic dodecahedrons. The atoms of the upper rhombic dodecahedron (indicated in Fig. 6 by solid circles) are two vertices of the RTID structure, and together with the corresponding atoms on the rear side of the dodecahedron form a square face of the RTID. The other vertices of the RTID are constructed in the same way. The length of all edges of this RTID is equal to $(2-2/\sqrt{5})^{1/2}$. The construction does not violate the matching rules[11] (indicated in Fig. 6 by line segment, triangle, and arrow). Therefore, the structure can exist in 3D PL's which, in an infinite system, again leads to the infinite degeneracy for the vertex model at $E=0$. In larger models structure of the localized states much richer than we observed in the models presented may be expected.

The strictly localized states that we have observed are a manifestation of the long-range bond-orientational order. The degeneracy of the energy level is the consequence of confinement (separability and independence) of

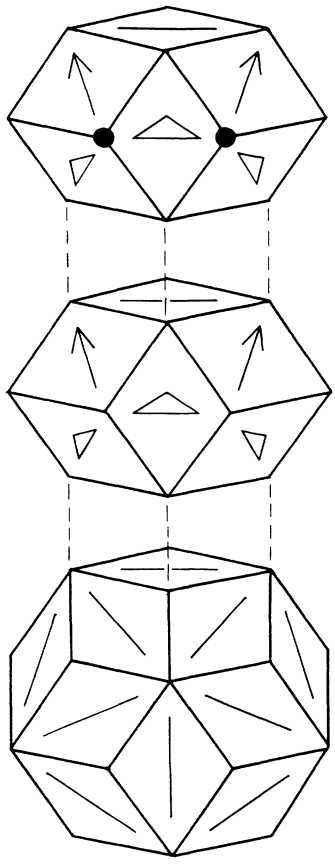

FIG. 6. The construction of the vertices (solid circles) of the rhombitriacontra icosidodecahedron which is topologically equivalent to that of Fig. 5. A rhombic triacontahedron in the center is covered by two layers of rhombic dodecahedra. The atoms indicated by the solid circles together with the equivalent atoms on the rear side of the upper rhombic dodecahedron form a square face of the RTID. The other vertices and faces are constructed in the same way. As the construction does not violate the matching rules (indicated by line segment, triangle, and arrow), such RTID can exist in the infinite Penrose lattice and cause the infinite degeneracy at $E=0$.

the localized states.

The infinitely degenerate states in the electronic spectrum of quasilattices were already observed in 2D models. In the 2D center model the degeneracy was observed for the first time by Semba and Ninomiya[13] and studied in detail by Fujiwara *et al.*[4] The degeneracy in the spectrum of the 2D vertex model was first reported by Kohomoto and Sutherland[5] and analyzed in detail by Arai *et al.*[6] Marcus[7] calculated the electronic structure of 2D and 3D vertex models on (3,2) PPL's. He could not find localized states and concluded that the electronic properties of quasilattices are little influenced by their quasiperiodic nature. At the present stage of this work, we cannot propose any statement about the possible singular continuous and multifractal structure of the electronic spectrum of 3D PL's similar to those observed in 1D and 2D quasiperiodic systems.[1–4]

The important property of a quasilattice is the long-range bond-orientational order. The long-range bond-orientational order and resulting local structure in real quasicrystals may give rise to strictly localized states similar to those we observed in our simple models and presumably others more complicated in larger or infinite models. The existence of such states in quasicrystals should manifest itself in an enhancement of the density of states and the resulting anomaly of physical properties such as electrical conductivity, electronic specific heat, etc. Particularly interesting should be physical properties of the system similar to our vertex model. If we consider one orbital per atom, the Fermi level lies just in the degenerate state $E=0$. If the localized states form an infinite connected structure, as in our (5,3) 3D PPL model, or consist of the infinite string states similar to those observed in 2D PL's, then, for instance, the conductivity of such a system should be extremely high.

V. SUMMARY

Structural models of the 3D periodic Penrose lattice have been constructed. The electronic structure of the center and vertex models was investigated. The degenerate levels in the electronic spectrum and the corresponding strictly localized states were found and analyzed.

ACKNOWLEDGMENTS

We thank T. Tokihiro for valuable discussions. One of us (M.K.) is also greatly indebted to the Japan Ministry of Education, Science and Culture (Monbusho) for providing financial support.

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*Permanent address: The Institute of Physics, Electro-Physical Research Center, Slovak Academy of Sciences, Dúbravská cesta 9, CS-842 28 Bratislava, Czechoslovakia.

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